

# Stripes: Why hole rich lines are antiphase domain walls?

Oron Zachar

ICTP, 11 strada Costiera, Trieste 34100, Italia

(February 1, 2008)

For stripes of hole rich lines in doped antiferromagnets, we investigate the competition between anti-phase and in-phase domain wall ground state configurations. We argue that a phase transition must occur as a function of the electron/hole filling fraction of the domain wall. Due to *transverse* kinetic hole fluctuations, empty domain walls are always anti-phase. At arbitrary electron filling fraction ( $\delta$ ) of the domain wall (and in particular for  $\delta \approx 1/4$  as in LaNdSrCuO), it is essential to account also for the transverse magnetic interactions of the electrons and their mobility *along* the domain wall.

We find that the transition from anti-phase to in-phase stripe domain wall occurs at a critical filling fraction  $0.28 < \delta_c < 0.30$ , for any value of  $\frac{J}{t} < \frac{1}{3}$ . We further use our model to estimate the spin-wave velocity in a stripe system. Finally, we relate the results of our microscopic model to previous Landau theory approach to stripes.

## I. INTRODUCTION

An anti-phase domain wall in stripes is the state where the local antiferromagnetic (AFM) spin order parameter undergo a  $\pi$  phase shift across a hole rich line. Such periodic stripe structures were experimentally found in doped Copper oxides and Nickel oxides [1]. Historically, this well accepted feature was first considered to be a natural outcome of mean-field theory Fermi surface instability [2,3]. Yet, no similar rigorous microscopic explanation was given within the frustrated phase separation picture [4] which is currently regarded as underlying the microscopic origin of stripes in the relevant materials [5]. One of our goals here is to close this gap in the theory.

In contrast with common folklore, we show that hole rich lines are not necessarily anti-phase domain walls of AFM spin domains. First, on simple general grounds, we argue that there must be a phase transition from anti-phase to in-phase domain wall configuration as a function of increased electron filling fraction  $\delta$  of the domain wall. We then proceed to construct microscopic t-J models of the local electronic dynamics which determines the resulting spin order across a hole line.

It is frequently argued theoretically [4,5] and exemplified experimentally [1] that the charge segregation into hole rich stripe lines is prior to the establishment antiphase spin domains. Therefore, the microscopic mechanism by which the hole lines enslave the spin order should be distinguished and considered separately.

We develop a qualitative and quantitative microscopic understanding of the domain wall magnetic order. Our analysis accounts for the electronic dynamics both transverse and along a pre-established hole rich line between two AFM domains. Thus we focus solely on the mechanism which give rise to the spin antiphase domain wall feature, by examining the competition between anti-phase and in-phase configurations at given electron filling fraction  $\delta$  of the hole rich line.

In the stripes literature it is more common to describe the domain wall filling in terms of the number of holes

(below half-filling) per site along the domain wall;

$$n^h = 1 - 2\delta. \quad (1)$$

Experimentally [1], anti-phase domain wall stripes in Nickel-Oxides have  $n^h \approx 1$  (corresponding to one hole per site along the domain wall, or equivalently an electron empty domain wall,  $\delta = 0$ ), while anti-phase domain wall stripes in Copper-Oxides have  $n^h \approx \frac{1}{2}$  (corresponding to one hole per two sites along the domain wall, or electron 1/4 filled domain wall,  $\delta \approx 0.25$ ). These domain wall filling fractions remain roughly constant over a wide range of dopings in the respective materials.

We find that the transition from anti-phase to in-phase stripe domain wall occurs at critical filling fraction

$$0.28 < \delta_c < 0.30 \quad (2)$$

depending on the value of  $(\frac{J}{t})$ . In other words, for example, we predict that stripe domain walls with a hole density of one hole per three sites are always in-phase and not anti-phase. Appropriate numerical simulations can be constructed to get exact numbers beyond the limits of our analytical approximations. Yet, since our analysis indicates that the sensitivity to  $(\frac{J}{t})$  is rather weak, we do not expect the exact numerical results to deviate much from our predictions.

We further apply our model to evaluate the of spin-wave velocity in a stripe systems, and compare with experiments. In addition, we relate the competing interactions in our microscopic model to previous Landau theory approach to stripes order [5,6]. Thus, we advance towards a coherent microscopic and phenomenological understanding of the stripes structure within the frustrated phase-separation picture.

## A. Overview of the model construction, analysis and main results

Since the paper is quite long, we here supply the reader with an overview of the gist of our model development

and main results.

The general intuitive argument for the domain wall transition is the following: In one extreme case,  $n^h = 1$ , where there is a hole on each site along the domain wall (i.e., it is empty of electrons,  $\delta = 0$ , as in Nickel-Oxides), it is clear that an anti-phase domain wall configuration is favored by transverse hole fluctuations. Now, consider the state of domain walls with increasing electron filling fraction. In the opposite extreme case where the domain wall is half-filled with electrons (i.e.,  $n^h = 0$ ,  $\delta = \frac{1}{2}$ ), we should recover the undoped ordered AFM state. Therefore, *there must be some intermediate critical electron filling fraction  $\delta_c$  of the domain wall at which there is a transition from an anti-phase to in-phase local AFM spin configuration across a hole rich line.*

The main quantitative objective of this paper is to determine the critical domain wall filling fraction  $\delta_c$  as a function of the t-J model parameters. In the process, we develop an advanced qualitative and quantitative understanding of the various competing local interactions in the single stripe physics. Additional applications are discussed in sections-V and VI.

Intuitively, increase of electron filling of the domain wall amounts to increase of magnetic interactions across the domain wall until they are strong enough to dominate over the charge fluctuation dynamics (due to holes). The possibility of a transition from topological (anti-phase) to non-topological (in-phase) stripes, due to increase of AFM interactions, was first speculated by Neto & Hone [7,8] (though, on not quite rigorous grounds, it was somehow related to the spin correlation length).

We find that the topological/non-topological nature of the stripe charge wall can be completely determined by the local dynamics, which in turn is determined by the electron filling fraction of the wall (assuming fixed given t-J model parameters). We do not see a way by which interaction between domain walls, the width of the spin domains or any similar long length scale are significantly relevant.

In section-II, we list some preliminary assumptions of our model of the stripe domain wall: (a) The effective electron dynamics is captured by a one band t-J model for electrons hopping between Copper sites (i.e., in which the Oxygen sites are integrated out). (b) It is assumed that the hole line, its mean position, and hole density are already pre-established by some higher energy processes (presumably phase separation and coulomb frustration). We hence focus solely on determining the preferred spin configuration across a pre-established hole line. (c) The spin order is determined by comparing the energetics of anti-phase and in-phase domain wall configurations (and not with the motion of dilute holes in a uniform AFM as was done in most previous work [9,10]).

In section-III, we introduce our microscopic model and start with the consideration of only *transverse* interactions and dynamics, (i.e., ignoring the effects of dynamics along the domain wall). The kinetic energy due to transverse hopping of holes favors an anti-phase domain

wall configuration, while magnetic interaction between electrons favors an in-phase domain configuration (see figure-1 below). These competing interactions determine the preferred local spin configuration. All calculations are done to the first significant order in  $(\frac{J}{t})$ . Our analysis surprisingly shows that if dynamics along the domain wall is ignored then transition to an in-phase domain wall would have occurred already at  $n^h \leq 2/3$  (i.e., at a density of two holes per three sites), in conflict with experimental observations of anti-phase stripes in *(LaNd)SrCuO* materials with  $n^h \approx 1/2$ . Hence, it is *essential* to investigate the effect of kinetic dynamics along the domain wall, which we undertake in section-IV.

In section-IV, we model the kinetic dynamics of the electrons moving along a stripe domain wall in an effective external magnetic mean field due to its AFM environment. Along an in-phase domain wall there is an effective net staggered external magnetic field, while along an anti-phase domain wall the net external field is zero on each site. We analyze two extreme limits: (a) Non-interacting electrons moving along the domain wall, and (b) Large  $U \gg t$  limit for the interaction of electrons along the domain wall. In both cases, the essential result is that kinetic fluctuations along the domain wall weaken the average magnetic interaction energy which favors an in-phase domain wall, and thus extend the stability of an anti-phase domain wall configuration to higher electron filling fractions (i.e., lower hole densities).

In section-V, we relate the competing interactions in our microscopic model to previous Landau theory approach to stripes order [5,6].

In section-VI, we apply our model to evaluate the spin-wave velocity  $v_\perp$  in a stripe state compared with  $v_0$  in the parent AFM material (where  $v_\perp$  is velocity perpendicular to the stripes).

We argue that our results are quantitatively accurate well beyond the seemingly rough approximations of our simple models. The heart of the matter is the fact that our quantitative results are sensitive only to the energetic *difference* between an anti-phase and in-phase domain wall configuration. Processes which are neglected in our treatment (e.g., deeper penetration of hole hopping into the AFM environment) have the same contribution in both domain wall configurations and thus only very weakly affect the energetic difference between them.

## II. PRELIMINARY ASSUMPTIONS

The stripes characteristics can vary to include both diagonal and vertical stripes, which may be insulating or conducting. Therefore, the anti-phase domain wall mechanism should be rather simple, robust, and not too sensitive to the above mentioned variations.

1. The most microscopic Hubbard type model of the  $\text{CuO}_2$  or  $\text{NiO}_2$  planes includes distinct Oxygen and

Copper (or Nickel) orbitals bands. Yet, as commonly argued, we assume that the effective dynamic is captured by a one-band t-J model [11] (in which the oxygen sites degrees of freedom have been integrated out) where electrons hop directly between Copper lattice sites. In the context of stripes theory, the above assumption is supported by the fact that correct domain wall configurations turned out in numerical simulations [12] of one band t-J models.

2. Experimental evidence [1] and theoretical considerations [5] suggest that stripe formation is commonly charge driven, i.e., that periodic hole line stripes form first and enslave the formation of the AFM spin domain. Therefore, for our purpose in this paper we take the hole lines to be pre-formed.
3. Stripes were found in both Spin- $\frac{1}{2}$  and Spin-1 doped antiferromagnets [1]. A doped hole can thus correspond to a spin-0 or a spin- $\frac{1}{2}$  site respectively. Yet, in both cases the hole and its dynamics are carried on only within the  $d_{x^2-y^2}$  orbital band. Indeed, the model which we construct and analyze works equally well for both doped Spin- $\frac{1}{2}$  and Spin-1 antiferromagnets. We chose to present our analysis in terms of a doped Spin- $\frac{1}{2}$  AFM (i.e., corresponding to stripes in a CuO<sub>2</sub> plane).
4. As with superexchange mechanism of antiferromagnetism in the undoped parent system, we argue that the domain wall spin order is determined by local interactions across the hole rich line. Hence, it is sufficient to consider a single stripe segment in isolation (see figure-1).
5. There's a non-trivial distinction between site-centered and bond-centered domain walls [13], in the sense that the spin alignment across an anti-phase domain wall is antiferromagnetic for site-centered stripe and ferromagnetic for bond-centered stripe. The presentation in this paper is conducted in terms of site-centered stripes, and elsewhere [14] we will show that the same principles apply for bond-centered stripes as well.
6. Probably the main quantitative approximation in our model is that we treat the AFM regions between the hole lines as if they were antiferromagnetically ordered. We neglect spin exchange fluctuations and the quantum nature of the AFM correlations in the rather narrow ladder geometry of the stripes. In other words, our quantitative results are rigorously valid for an Ising model approximation of the AFM regions. Yet, in all of our calculations we use a parameter  $\varepsilon$  which is defined to be the energy difference between parallel and anti-parallel near-neighbor spin states (see equation (5)). Only in the end we substitute  $\varepsilon = J$  for intuitive concreteness. In principle, all the effects of fluctuations

etc. can be incorporated into a renormalized value of  $\varepsilon$  without changing our results.

7. Our quantitative results are sensitive only to the energetic *difference* between an anti-phase and in-phase domain wall configuration. Therefore, many processes which are neglected in our treatment (e.g., deeper penetration of hole hopping into the AFM environment, magnetic interaction between electrons on the wall) have the same contribution in both domain wall configurations and thus only very weakly affect the energetic difference between them.

### III. THE EFFECT OF TRANSVERSE INTERACTION

Our analysis proceed in two stages; First, in this section, we consider solely the *transverse* fluctuations of a hole and magnetic interaction of electrons in the stripe, while the holes/electrons configuration along the domain wall is taken as static. In a second stage (section-IV), we consider the implications of electron mobility *along* the stripe.

#### A. Model of site-centered stripe

The average hole line position is fixed by introducing a chemical potential shift ( $\mu$ ) on particular sites [7,8]. (In Figure-1, hole line  $\mu$ -shifted sites are represented by dark circles). In the ground state, holes are preferentially situated on the  $\mu$  shifted sites. Hence, the effective local chemical potential shift,  $\mu$ , incorporates the net effect of the high energy dynamics (e.g., coulomb frustrated phase separation [4]) which lead to the stripe formation. The magnitude of  $\mu$  determines the stripe stability, and can be associated with the stripe creation temperature for the purpose of extracting an experimental estimate of it's magnitude. Thus, it is assumed that  $\mu < J < t$ .

An antiferromagnetic spin exchange interaction  $J$  exists between electron spins on nearest neighbors sites. In order to fix the spin order, it is enough to determine the relative orientation of the spins immediately to the left and to the right of the hole line. Therefore, we include a *transverse* hopping interaction,  $t$ , only between a domain wall site (indicated by a dark circle in figure-1a) and its right and left nearest neighbors in the AFM regions. As noted before, we argue that processes of further penetration of a hole into the AFM regions are not significantly affecting our results. Hopping interaction  $t_{\parallel}$  *along* the domain wall will be considered in section-IV.

In the absence of kinetic motion along the domain wall, the Hamiltonian describing a single site centered domain wall is

$$H = \sum_i H_i \quad (3)$$

$$H_i = \mu n_{0,i} + J \frac{1}{2} \sum_{\langle jj' \rangle \langle ii' \rangle} \mathbf{S}_{j,i} \cdot \mathbf{S}_{j',i'} \quad (4)$$

$$-t \sum_{i,s} \left[ \left( c_{1,i,s}^\dagger c_{0,i,s} + c_{-1,i,s}^\dagger c_{0,i,s} \right) + \text{h.c.} \right]$$

where  $\mathbf{S}_{j,i}$  is the spin of an electron at column  $j$  and line  $i$  (where  $j = 0$  is the domain wall position).  $n_{0,i}$  is the occupation number of a domain wall site at position  $i$  along the wall.  $c_{1,i,s}^\dagger$  and  $c_{-1,i,s}^\dagger$  are electron creation operators respectively to the right and left of the domain wall site  $n_{0,i}$ . (t-J model projection operator which excludes double occupancy is implicitly assumed throughout the paper).

### B. Kinetic transverse hole fluctuations

In the absence of hopping interaction,  $t$ , the anti-phase stripe groundstate (a) and the in-phase stripe groundstate (a') are degenerate. But, the energy of the corresponding excited states (b) and (b') differ. As a result, *transverse hole hopping interaction removes the ground state degeneracy in favor of anti-phase domain wall* [15].

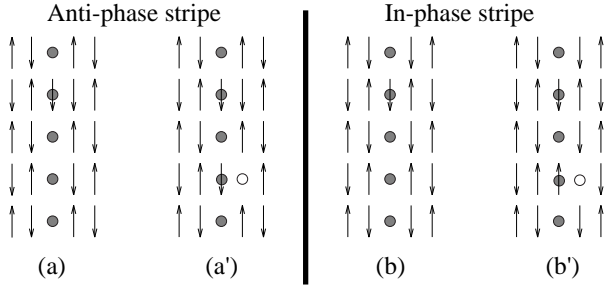


FIG. 1. The domain wall sites are indicated by colored circles. The static ground state configuration of anti-phase and in-phase domain walls are depicted in figures (a) and (b) respectively. The corresponding excited states (a') and (b') result from transverse hopping dynamics of holes. Note the "bad bond" created by the hopping in (b'). The depicted domain wall groundstate segments have one electron per 5 sites on the domain wall (i.e., a filling fraction  $\delta^e = 0.1$ ). Note the difference in the magnetic bonds of the domain wall electron between (a) and (b).

To be general, we define  $\varepsilon$  to be the energy difference between an antiferromagnetic "good bond" and a ferromagnetic "bad bond" of two neighboring spins. Obviously,  $\varepsilon$  is proportional to  $J$  (and  $\varepsilon = J$  in the case of Ising model of the AFM spin domains). We label by  $E_1^{anti}$  and  $E_1^{in}$  the bare excited states energy in the case of an anti-phase and in-phase domain walls as depicted in figure (1b) and (1b') respectively. Clearly,

$$E_1^{in} - E_1^{anti} = \varepsilon \quad (5)$$

The Hamiltonian (4) is thus given by the matrix

$$H^\alpha = \begin{pmatrix} 0 & t & t \\ t & E_1^\alpha & 0 \\ t & 0 & E_1^\alpha \end{pmatrix} \quad (6)$$

( $\alpha = \text{anti/in}$ ) which can be diagonalized exactly, resulting with the ground state energy  $E_g^\alpha$

$$E_g^\alpha = \frac{1}{2} \left( E_1^\alpha - \sqrt{(E_1^\alpha)^2 + 8t^2} \right) \quad (7)$$

$$\approx \begin{cases} \frac{1}{2} \left[ E_1^\alpha - \sqrt{8}t \left( 1 + \frac{(E_1^\alpha)^2}{16t^2} \right) \right] & \text{for } J \ll t \\ -\frac{2t^2}{E_1^\alpha} & \text{for } J \gg t \end{cases}$$

The difference in kinetic energy gain due to transverse hopping, between an anti-phase and an in-phase domain wall configurations, is given by

$$\Delta E_1^{kin} = E_g^{anti} - E_g^{in} \quad (8)$$

$$\approx \begin{cases} -\frac{\varepsilon}{2} + \mathcal{O}\left(\frac{\varepsilon^2}{t}\right) & \text{for } J \ll t \\ -\frac{t^2}{\varepsilon} & \text{for } J \gg t \end{cases} \quad (9)$$

Our result agrees with a previous large-d calculation (valid only in the limit  $J \gg t$ ) [16]. But, in the experimental systems of interest  $\frac{J}{t} \approx \frac{1}{3}$ , and thus they are better approximated by calculations in the limit  $J \ll t$  which will be assumed for the rest of our discussion. From equation (8) we conclude that, *in a site-centered stripe geometry, the zero point transverse kinetic fluctuation of the holes favor an antiferromagnetic alignment of the neighboring spins.*

Note that the above result is in stark contrast with the conventional wisdom that hole's zero-point kinetic fluctuations always favors ferromagnetic alignment of their environment [17,18], which is based mostly on isolated hole models. It is a rather simple demonstration of the difference between collective and single hole properties in doped antiferromagnets.

### C. Competing magnetic interactions at electron filling $\delta \neq 0$

From the analysis of the above model, we conclude that *the transverse kinetic fluctuations of holes are sufficient to induce an anti-phase domain wall ground state in an empty domain wall  $\delta = 0$  (i.e., one hole per site along the wall,  $n^h = 1$ ) of stripes.*

For a domain wall with electron filling fraction of  $\delta$ ,  $2\delta$  is the number of electrons per site along the domain wall (in the large  $U$  limit), and  $n_h = (1 - 2\delta)$  is the number of holes in the lower Hubbard band. Each hole contributes a kinetic energy difference  $\Delta E_1^{kin}$ . Hence, at an arbitrary electron filling fraction  $\delta$  of the domain wall, the average *transverse kinetic energy gain per site*  $\Delta E_\perp^{kin}(\delta)$  of an anti-phase domain wall in comparison with an in-phase domain wall is

$$\Delta E_{\perp}^{kin}(\delta) = \frac{\Delta E_1^{kin}}{N_{site}} = -\frac{\varepsilon}{2}(1-2\delta) \quad (10)$$

For each electron on the domain wall there is an energy difference  $\Delta E_1^{mag} = +\varepsilon$  in favor of an in-phase domain wall, due to spin exchange interaction with the AFM environment. At electron filling  $\delta$ , the average magnetic energy difference (of an anti-phase domain wall in comparison with an in-phase domain) per site along the domain wall is

$$\Delta E_{\perp}^{mag}(\delta) = \frac{\Delta E_1^{mag}}{N_{site}} = +\varepsilon(2\delta). \quad (11)$$

*The competition of these transverse interaction alone would predict a transition as a function of domain wall filling from anti-phase to in-phase domain wall when*

$$\Delta E_{\perp}(\delta) = \Delta E_{\perp}^{kin} + \Delta E_{\perp}^{mag} > 0 \quad (12)$$

at

$$\delta \geq \frac{1}{6} \quad (13)$$

(corresponding to  $n^h \leq 2/3$ , i.e., at a density of two holes per three sites), in conflict with experimental observations of anti-phase stripes in  $(LaNd)SrCuO$  materials with  $\delta \approx 1/4$ . This conflict is resolved in the next section, where we account for effect of kinetic dynamics along the domain wall.

#### IV. IMPLICATIONS OF ELECTRON DYNAMICS ALONG THE DOMAIN WALL

In this section we investigate the consequences of electron dynamics along the domain wall for the competition between anti-phase and in-phase domain wall configurations. As a first order approximation, we assume static spin configuration of the antiferromagnetic domains on the left and right of the domain wall. Thus, electrons moving along the domain wall are effectively modeled as a one-dimensional electron gas (1DEG) in a static external magnetic field. At this mean-field level, electrons moving in an anti-phase domain wall experience a net zero external field on each site, while electrons moving on an in-phase domain wall experience a staggered external magnetic field of magnitude proportional to the spin interaction strength  $J$ . Hence, the effective domain wall 1DEG Hamiltonian has the form

$$H = H_0(B) + U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (14)$$

$$H_0(B) = t_{\parallel} \sum_{j\sigma} \left( c_{j\sigma}^{\dagger} c_{j+1,\sigma} + h.c. \right) - \mu_F \sum_{j\sigma} c_{j\sigma}^{\dagger} c_{j\sigma} + 2B \sum_{j\sigma} \sigma (-1)^j c_{j\sigma}^{\dagger} c_{j\sigma} \quad (15)$$

where  $\sigma = \pm 1$  for spin  $\uparrow, \downarrow$  respectively, and

$$B = \begin{cases} 0 & \text{for anti-phase} \\ \approx \frac{J}{4} & \text{for in-phase} \end{cases} \quad (16)$$

When considering the competition of stripes versus droplets forms of local phase separation, Nayak&Wilzek [9] proposed that a significant energy is gained by the increased mobility *along* an anti-phase domain wall. But we note that the kinetic energy gain in an in-phase domain wall is practically the same as in anti-phase domain wall state. Therefore, it is essential to make a more careful analysis of the electronic dynamics along the domain wall in both cases.

Below, we extract quantitative results in two limits: (a) For non-interacting electrons moving along the domain wall, and (b) In the large  $U \gg t$  limit for the interaction of electrons along the domain wall. In both cases, the essential result is that kinetic fluctuations along the domain wall weakens the magnetic interaction energy gain which favors an in-phase domain wall environment, and thus extends the stability of anti-phase domain wall configuration to higher electron filling fractions (i.e., lower hole densities). In particular, we conclude that dynamics fluctuations along the domain wall allow for the establishment of anti-phase stripes with domain wall filling  $\delta \approx \frac{1}{4}$  (as in Copper-Oxides systems).

##### A. Effect of motion along the domain wall for non-interacting electrons at arbitrary filling

We here model the dynamics along the hole rich domain wall by an effective one dimensional lattice model (14) of non-interacting electrons ( $U = 0$ ). For an in-phase domain wall, the exchange coupling to the spins in the AFM environment result with an effective external staggered magnetic field on the electrons moving along the domain wall (see figure-1b). Our model of kinetic motion along the domain wall included only band structure effects due to a static spin configuration of the AFM environment, but no dynamic scattering interactions (leading to finite resistivity) [19].

The anti-phase domain wall spectrum ( $B = 0$ ) is

$$E_n^{(anti)} = -2t_{\parallel} \cos(k_n a) - \mu_F^{(anti)} \quad (17)$$

$$k_n a = \frac{2\pi}{N} n \quad \left( -\frac{N}{2} \leq n \leq \frac{N}{2} \right) \quad (18)$$

$$\mu_F^{(anti)} = -2t_{\parallel} \cos\left(\frac{2\pi}{N} n_F\right) \quad (19)$$

where  $N$  is the number of sites.

For an in-phase domain wall ( $B \neq 0$ ), the staggered field doubles the unit cell. The non-interacting Hamiltonian (15)  $H_0(B \neq 0)$  is diagonalized by the appropriate Bloch states;

$$\psi_{k,\sigma}^\dagger = \sqrt{\frac{2}{N}} \sum_{j=1}^{N/2} e^{+ik(2ja)} W_{j,\sigma}(k) \quad (20)$$

$$W_{j,\sigma}(k) = \frac{1}{\sqrt{1 + |f_{k,\sigma}|^2}} \left[ c_{2j,\sigma}^\dagger + f_{k,\sigma} e^{-ika} c_{2j-1,\sigma}^\dagger \right]$$

$$f_{k,\sigma} = \frac{-\sigma \left(\frac{B}{t}\right) \mp \sqrt{\left(\frac{B}{t}\right)^2 + \cos^2(k)}}{\cos(k)}$$

The resulting energy spectrum for the in-phase domain wall is

$$E_n^{(in)} = \pm 2t_\parallel \sqrt{\left(\frac{B}{t_\parallel}\right)^2 + \cos^2\left(\frac{2\pi}{N}n\right)} - \mu_F^{(in)} \quad (21)$$

$$\left(-\frac{N}{4} \leq n \leq \frac{N}{4}\right) \quad (22)$$

$$\delta = \frac{2n_F}{N} \quad (23)$$

In this context we comment that for a Hubbard model in an external staggered magnetic field, unlike the case of staggered charge potential/interaction, there is no charge gap opening at  $1/4$  filling [14]. For simplicity, the rest of the formulas are written for the case where the odd-sites are with the magnetic field anti-parallel to the spin. Moreover, we remind the reader that we assume  $B \sim J \ll t_\parallel$ . Well below half filling, (i.e.,  $t_\parallel \cos(k) > 0$ ),

$$f_{k,\uparrow} = \frac{-B + \sqrt{B^2 + t_\parallel^2 \cos^2(k)}}{t_\parallel \cos(k)} \approx 1 - \frac{B}{t_\parallel \cos(k)} + \mathcal{O}\left(\frac{B}{t_\parallel \cos(k)}\right)^2 \quad (24)$$

The gain in magnetic energy per  $k$ -state is due to the difference between the occupation probability of odd and even sites for a given electron spin, (this is the main difference between 1DEG in an in-phase vs. anti-phase domain wall),

$$\begin{aligned} & \left| \left\langle c_{2j,\sigma}^\dagger c_{2j,\sigma} \right\rangle_k \right|^2 - \left| \left\langle c_{2j-1,\sigma}^\dagger c_{2j-1,\sigma} \right\rangle_k \right|^2 \\ & \approx \sum_{j=1}^{N/2} \frac{2}{N} \frac{1}{1 + |f_{k,\sigma}|^2} \left( 2 \frac{B}{t_\parallel \cos(k)} \right) \\ & \approx \left( \frac{B}{t_\parallel \cos(k)} \right) + \mathcal{O}\left(\frac{B}{t_\parallel \cos(k)}\right)^2 \end{aligned} \quad (25)$$

Therefore, for filling up to  $k_F$ , the magnetic interaction energy gain for an in-phase domain wall in comparison with an anti-phase domain wall is given approximately by,

$$\Delta E^{mag}(\delta) \approx 2B \left[ 2 \int_{-\pi\delta}^{\pi\delta} \frac{B}{t_\parallel \cos(k)} dk \right] \quad (26)$$

$$= 2B \left[ 2 \left( \frac{B}{t_\parallel} \right) \ln \left( \frac{1 + \sin(\pi\delta)}{1 - \sin(\pi\delta)} \right) \right] \quad (27)$$

$$\approx \frac{J}{4} \left[ \frac{J}{t_\parallel} \ln \left( \frac{1 + \sin(\pi\delta)}{1 - \sin(\pi\delta)} \right) \right] \quad (28)$$

(Note that the limit  $t_\parallel \rightarrow 0$  of the previous section cannot be recovered since we used approximations based on  $t_\parallel \gg B \approx J/4$ ).

We are now in a position to give a first analytical estimate of the critical transition point filling  $\delta_c$  determined given by (using (10) and (28))

$$0 = \Delta E_\perp(\delta_c) \approx E_\perp^{kin} + \Delta E^{mag} \quad (29)$$

$$\approx -\frac{J}{2} (1 - 2\delta_c) + \frac{J}{4} \left[ \frac{J}{t} \ln \left( \frac{1 + \sin(\pi\delta_c)}{1 - \sin(\pi\delta_c)} \right) \right] \quad (30)$$

The geometrical solution for  $\frac{J}{t} = \frac{1}{3}, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \frac{1}{10}$  is plotted in figure-2

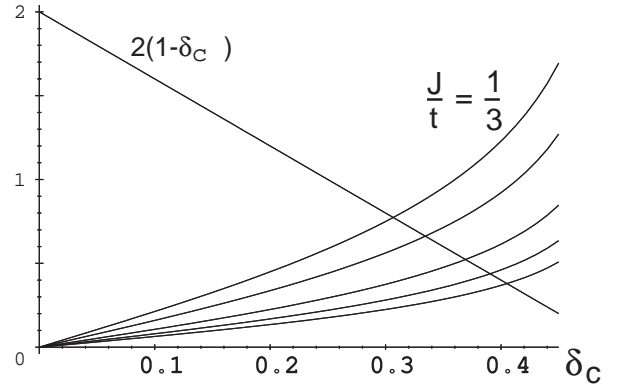


FIG. 2. geometrical solution for  $\frac{J}{t} = \frac{1}{3}, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \frac{1}{10}$

The main qualitative result is that *electron hopping fluctuations along a partially filled domain wall inhibit the effective magnetic interaction energy across the domain wall*. As a result, an anti-phase domain wall ground-state configuration can be obtained beyond  $\delta = \frac{1}{6}$ , depending on the value of  $J/t$ . For  $\frac{1}{3} \leq \frac{J}{t} \leq \frac{1}{10}$  we find  $0.3 < \delta_c < 0.4$ . Note that the critical filling fraction  $\delta_c$  is not very sensitive to the value of  $J/t$ . Most importantly, it is above the value  $\delta \approx 0.25$  of anti-phase stripes in  $(LaNd)SrCuO$  systems [1].

## B. Large $U \gg t$ model, and a second estimate of the critical domain wall filling $\delta_c$

In this subsection we examine the competition between anti-phase and in-phase domain wall configurations for

strongly interacting electrons,  $U \gg t$ , along the domain wall at arbitrary filling fraction.

The exact ground-state energy of the Hubbard model (14) is well known for the case  $B = 0$  from Bethe ansatz solution. Unfortunately, we do not know of an established solution for the groundstate energy of a one dimensional Hubbard model in a staggered magnetic field  $B \neq 0$ . In particular, when  $B = 0$  the Hubbard interaction in momentum space takes the form  $U n_{k\uparrow} n_{k\downarrow}$ , and the  $U = \infty$  limit is effectively captured by imposing a restriction of one electron per  $k$ -state. But such a simple representation does not exist in terms of the  $W_{j,\sigma}(k)$  basis (20) in a staggered external magnetic field. Therefore, we here develop a way to approximate the two competing wall configuration energies at the same level of approximation.

We wish to stress that the qualitative effect of longitudinal hopping fluctuations - to inhibit the effective magnetic interaction energy across the domain wall - was already established in the preceding subsection. The purpose of the current subsection is to investigate the quantitative effect of including large Hubbard interactions between the electrons. Though we indeed resort to approximations at several stages of our model and calculations, we do capture the substantial effect. Once the core physics established, the degree to which our final numerical values are exact can be checked (and improved) in numerical simulations on finite systems.

Our main result is that the *large Hubbard interaction*,  $U$ , *delimitate the critical filling fraction to be in the narrow range*

$$0.28 < \delta_c < 0.30 \quad (31)$$

for any value of  $\frac{J}{t} < \frac{1}{3}$ .

Below, we explain our modeling approach and calculation. We first apply the model to examine the simplest case of  $1/4$  filled domain wall, and show that always an anti-phase is obtained. Then, we apply the model to re-estimate the critical filling fraction for a transition to an in-phase domain wall, and thus establish the result noted above in equation (31).

### 1. Model of characteristic unit cells

The unit cell of a stripe domain wall comprise of two lines as depicted in figure-3. Our modeling idea in this subsection is to *solve exactly the Hamiltonian of isolated prototypical unit cells, and then approximate the full stripe as assembled of a collection of such unit cells*. Such an approximation is building on our findings in the previous subsection, where we argued that it is not the global longitudinal mobility, but only the local kinetic fluctuations (in the occupation of odd/even numbered sites along the wall) which distinguish anti-phase and in-phase domain walls.

As shown in figure-3, in the  $U = \infty$  limit, there are only three possible electron occupation numbers of a unit cell: one, two or zero electrons on the domain wall sites. In our model approximation, we ignore the hopping from one unit cell to another. As we shall later explain, for filling fractions  $\delta \geq \frac{1}{4}$  it will suffice to consider only unit cells with one and two electrons on the domain wall sites (i.e., as in figure-3(a1,a2 and b1,b2)).

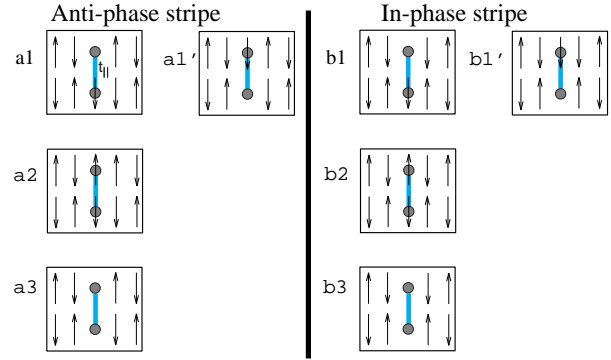


FIG. 3. Characteristic unit cells of a stripe domain wall. Any domain wall groundstate can be constructed by properly assembling these unit cells. For domain wall groundstate with filling fraction  $\delta^e > 1/4$ , unit cells (a3) and (b3) can be neglected.

We are interested only in the effect of hopping dynamics  $t_{\parallel}$  of electron along the domain wall. Therefore we examine first the unit cells with one hole and one electron on the domain wall sites. There's spin exchange interactions of strength  $J$  between nearest-neighbor electrons. Yet, to zeroth level of approximation, the spin configuration is assumed to be static (apart from  $t_{\parallel}$  electron hopping). Thus, we consider only the electron configurations of an anti-phase (a1,a1') and in-phase (b1,b1') domain wall unit cells.

Consider the case of unit cells with a single hole and spin- $\downarrow$  electron hopping between the domain wall sites. We observe that while the anti-phase domain wall states (a1,a1') are degenerate, the in-phase domain wall states (b1 and b1') have an energy difference of magnitude  $2\varepsilon$  (where  $\varepsilon \sim J$  is the energy difference between parallel and anti-parallel neighboring spin states). Thus, the Hamiltonian of a single electron in an anti-phase domain wall unit cell is

$$H_{\text{hole-cell}}^{\text{anti}} = \begin{pmatrix} 0 & -t_{\parallel} \\ -t_{\parallel} & 0 \end{pmatrix} \quad (32)$$

with groundstate energy  $-t$ , while for an in-phase domain wall

$$H_{\text{hole-cell}}^{\text{in}} = \begin{pmatrix} -\varepsilon & -t_{\parallel} \\ -t_{\parallel} & +\varepsilon \end{pmatrix} \quad (33)$$

with groundstate energy  $-\sqrt{\varepsilon^2 + t_{\parallel}^2} \approx -\left[t_{\parallel} + \frac{1}{2}\left(\frac{\varepsilon}{t_{\parallel}}\right)\varepsilon\right]$ . (Note that the magnetic interaction energy is already fully accounted for in

the eigenvalues, so it shouldn't be counted again). Thus we find that, for a stripe unit cell with one hole and one electron on the domain wall sites, the ground state magnetic interaction energy difference between an anti-phase and in-phase domain wall is

$$\begin{aligned}\Delta E_{\text{hole-cell}}^{\text{mag}} &= E_{\text{hole-cell}}^{\text{anti}} - E_{\text{hole-cell}}^{\text{in}} \\ &= -t_{\parallel} + \sqrt{(\varepsilon^2 + t_{\parallel}^2)} \\ &\approx \begin{cases} +\frac{1}{2} \left( \frac{\varepsilon}{t_{\parallel}} \right) \varepsilon & \text{for } t_{\parallel} \gg J \\ +\varepsilon & \text{for } t_{\parallel} \rightarrow 0 \end{cases}\end{aligned}\quad (34)$$

The above needs to be divided by 2 in order to get the energy difference per site, since the unit cell has two sites along the domain wall. In the static limit  $t_{\parallel} \rightarrow 0$ , we recover equation (11) of section-III,  $\frac{\Delta E_{\text{hole-cell}}^{\text{mag}}(\delta=1/4)}{N} \approx +\frac{\varepsilon}{2}$ . But for the rest of the paper, we focus on the experimentally more relevant limit  $t_{\parallel} \gg J$ .

We now proceed to demonstrate first the essence of our approach for the simplest case of  $\delta = \frac{1}{4}$  filling.

## 2. The special case of $1/4$ filling

In section-III, we have shown that dynamics of only *transverse* interactions (hole hopping and Heisenberg interaction) will not suffice to stabilize an anti-phase domain wall for  $\delta > 1/6$ . Therefore, by investigating the case of  $\delta = 1/4$  we can already answer the question of principle about the effect of electron dynamics *along* a stripe domain wall. Moreover, it is a case of particular interest for stripes in HTc, which are found with a filling fraction very near  $\delta = 1/4$ .

In the limit of large on-site interaction  $U \gg t$ , at  $\delta = 1/4$  there is effectively one electron for every two sites along the wall. Moreover, to mimic the expected effect of coulomb interactions, it makes sense to supplement the model with a repulsive interaction also between near-neighbor holes (i.e., a  $t - U - V$  model along the domain wall) [20]. Thus, in the absence of kinetic hopping dynamics along the domain wall, the groundstate of the one dimensional electron gas is a periodic charge density wave (CDW) with one electron per every second site. Even with the inclusion of kinetic fluctuations, the same CDW still dominate the electron correlations at low temperatures. As a result, we argue that the occurrence of unit cells with an occupation of zero or two electrons on the domain wall sites (as in figure-3(a2,a3)) are rare events and thus their contribution may be safely neglected.

Therefore, a two-line stripes segment with one hole and one electron on the domain wall sites can be regarded as the characteristic unit cell along a  $1/4$  filled domain wall (as in figure-3(a1,b1)). By solving such unit cell model exactly, we are able to account for the effect of local kinetic fluctuations along the domain wall. Moreover, since we are interested only in the difference between

anti-phase and in-phase wall, and since the net magnetic field averages to zero along both anti-phase and in-phase wall, it is intuitively expected that *the significant difference is not in the net electron mobility but mostly in the local kinetic fluctuations* (Though magnetic scattering from AFM environment, which we neglect, may also differ).

Let us recall first the result of section-III. In the absence of hopping along the wall, the average transverse kinetic energy per site of an anti-phase domain wall in comparison with an in-phase domain wall was (using equation (10))

$$\Delta E_{\perp}^{\text{kin}} \left( \delta = \frac{1}{4} \right) = \frac{E_{\perp}^{\text{kin}}}{N} = -\frac{\varepsilon}{2} (1 - 2\delta) = -\frac{\varepsilon}{4}$$

and the competing transverse magnetic energy due to Heisenberg interaction with the AFM environment was (using equation (11))

$$\Delta E_{\perp}^{\text{mag}} \left( \delta = \frac{1}{4} \right) = \frac{E_{\perp}^{\text{mag}}}{N} = +\varepsilon (2\delta) = +\frac{\varepsilon}{2}.$$

Hence, it was the in-phase domain wall configuration which had the lowest energy ground state. Now, with the inclusion of the effect of the kinetic fluctuations along the domain wall, the average magnetic interaction energy is modified and (using (34) instead of (11)) the average energy difference per site is

$$\frac{\Delta E}{N} = \Delta E_{\perp}^{\text{kin}} + \frac{1}{2} \Delta E_{\text{hole-cell}}^{\text{mag}} \quad (35)$$

$$\frac{\Delta E(\delta = 1/4)}{N} \approx -\frac{\varepsilon}{4} + \left( \frac{\varepsilon}{t_{\parallel}} \right) \frac{\varepsilon}{4} < 0 \quad (36)$$

where  $N$  is the number of sites along the domain wall, (The factor  $1/2$  in (35) is due to having two domain wall sites per unit cell). Therefore, we find that due to the kinetic fluctuations along the domain wall, the magnetic interaction energy gain of an in-phase domain wall configuration is reduced enough to make the anti-phase domain wall more favorable at  $1/4$  filling for any value of  $J \sim \varepsilon < t_{\parallel}$ .

## 3. Transition at domain wall filling $\delta_c$

We now attempt to determine the contribution of the effect described above at arbitrary electron filling  $2\delta > \frac{1}{2}$ , and thus estimate the transition point.

As argued before, the 1DEG correlations on the domain wall are dominated by a CDW correlations where, at electron filling  $2\delta > 1/2$ , the occurrence of two near-neighbor holes is statistically negligible compared with other configurations in the ground state. Therefore, the two-sites unit cells along the domain wall are basically only of two kinds: (a) There are  $(1 - 2\delta)$  unit cells containing one hole, which are the type analyzed in the previous subsection. (b) There are  $\frac{1}{2} - (1 - 2\delta) = (2\delta - \frac{1}{2})$  unit cells containing no holes.



To estimate the average energy contribution per site, we can use the result of the previous subsection for the hole cells, only with the added factor  $(1 - 2\delta)$ ;

$$\Delta E^a(\delta) = \Delta E_{\perp}^{kin} + \frac{1}{2} \Delta E_{\text{hole-cell}}^{mag} \quad (37)$$

$$= -\frac{\varepsilon}{4} \left[ 1 - \left( \frac{\varepsilon}{t_{\parallel}} \right) \right] (1 - 2\delta) \quad (38)$$

and add the contribution of magnetic energy difference per site due to unit cells with no holes,

$$\Delta E^b(\delta) = \frac{1}{2} E_{2e\text{-cell}}^{mag} = +\frac{1}{2} \left( 2\delta - \frac{1}{2} \right) 2\varepsilon. \quad (39)$$

The preferred groundstate configuration is determined by

$$\frac{\Delta E(\delta)}{N} = \Delta E^a(\delta) + \Delta E^b(\delta) \quad (40)$$

$$= -\frac{\varepsilon}{4} \left[ 1 - \left( \frac{\varepsilon}{t_{\parallel}} \right) \right] (1 - 2\delta) + \left( 2\delta - \frac{1}{2} \right) \varepsilon. \quad (41)$$

A transition from anti-phase to in-phase domain wall occurs when

$$\Delta E(\delta) > 0$$

Therefore, the critical filling fraction  $\delta_c$  is given by

$$0 = -\frac{\varepsilon}{2} \left[ 1 - \left( \frac{\varepsilon}{t_{\parallel}} \right) \right] (1 - 2\delta_c) + 2 \left( 2\delta_c - \frac{1}{2} \right) \varepsilon \quad (42)$$

$$\delta_c = \frac{\frac{3}{2} - \frac{1}{2} \left( \frac{\varepsilon}{t_{\parallel}} \right)}{5 - \left( \frac{\varepsilon}{t_{\parallel}} \right)} \quad (43)$$

The predicted  $\delta_c$  for several values of  $\frac{\varepsilon}{t}$  is given below,

$$\delta_c \left( \frac{\varepsilon}{t} = \frac{1}{3} \right) = 0.28571$$

$$\delta_c \left( \frac{\varepsilon}{t} = \frac{1}{6} \right) = 0.2931$$

$$\delta_c \left( \frac{\varepsilon}{t} \rightarrow 0 \right) \lesssim 0.3$$

We find that  $0.28 < \delta_c < 0.3$ , (for  $\frac{J}{t} < \frac{1}{3}$ ), and is only weakly sensitive to the value of  $\frac{J}{t}$ .

## V. CONNECTION WITH A LANDAU THEORY OF STRIPES ORDER

The properties of a general Ginzburg-Landau free energy (44) of stripes were previously investigated in [5,6]. Specifically, an ordered stripe phase is a unidirectional density wave which consists of coupled spin-density wave (SDW) and charge-density wave (CDW) order parameters.

$$\mathcal{F}_{q,k} = r_{1s} |\mathbf{S}_{\vec{q}}|^2 + r_{2s} \left| \mathbf{S}_{\vec{q}+\vec{k}} \right|^2 + r_c |\rho_{\vec{k}}|^2 \quad (44)$$

$$+ \gamma \left[ \mathbf{S}_{\vec{q}}^* \mathbf{S}_{\vec{q}+\vec{k}} \rho_{\vec{k}}^* + \text{c.c.} \right] + \dots,$$

where  $\rho_{\vec{k}}$  is the complex-valued CDW amplitude with wave vector  $\vec{k}$ ,  $\rho_{\vec{k}}^* \equiv \rho_{-\vec{k}}$ , and similarly  $\mathbf{S}_{\vec{q}}$  is a complex vector amplitude of the SDW. The quartic (and higher order) terms required for stability are omitted.

Zachar *et al.* [5] have considered the phase transition between a stripe phase and a high-temperature disordered state, as involving only a *single SDW wave vector* (i.e.,  $\mathbf{S}_{\vec{q}}^* = \mathbf{S}_{\vec{q}+\vec{k}}$ ). The existence of the cubic  $\gamma$  term, coupling these two order parameters in the Landau free energy, drives the period of the SDW to be twice that of the CDW, and the absence of any net AFM ordering is equivalent to the statement that the stripes are topological.

In contrast, it was shown by Pryadko *et al.* [6], that the same sort of cubic term in a Landau theory of the transition from a homogeneous ordered antiferromagnetic phase to a stripe ordered phase produces a state in which the antiferromagnetic magnetization *does not* change its sign between the domains, i.e. the stripes are non-topological.

When investigating the transition from a well-developed antiferromagnet with a modulation vector  $\vec{\pi} = (\pi, \pi)$  to an incommensurate modulated phase, we must account for both the original AFM order parameter  $\mathbf{S}_{\vec{\pi}}$  (which cannot be assumed small), and the spin density wave  $\mathbf{S}_{\vec{\pi}+\vec{k}}$ . The most relevant terms in the Landau expansion of the effective free energy are then

$$\mathcal{F} = r_{1s} |\mathbf{S}_{\vec{\pi}}|^2 + r_{2s} \left| \mathbf{S}_{\vec{\pi}+\vec{k}} \right|^2 + r_c |\rho_{\vec{k}}|^2 \quad (45)$$

$$+ \gamma \left[ \mathbf{S}_{\vec{\pi}}^* \mathbf{S}_{\vec{\pi}+\vec{k}} \rho_{\vec{k}}^* + \text{c.c.} \right] + \dots,$$

where a finite  $r_{1s} < 0$  is assumed as given. This expression implies that an instability in either spin or charge sector generates both spin- and charge-density waves at the wave vectors  $\vec{q} = \vec{\pi} + \vec{k}$  and  $\vec{k}$ , respectively. Near the transition the magnitude of the incommensurate peak is necessarily much smaller than the commensurate AFM modulation  $|\mathbf{S}_{\vec{\pi}+\vec{k}}| \ll |\mathbf{S}_{\vec{\pi}}|$ . It is easy to see that this corresponds to *in-phase* domain walls; The derived relationship between  $\vec{q}$  and  $\vec{k}$  implies that the periods of spin and charge modulation are equal.

Our analysis in this paper supply microscopic insight to the Landau theory results. First, we find that the possibility of both topological and non-topological stripe phases can indeed be realized within a single microscopic model (as anti-phase and in-phase domain wall ground-states respectively).

Second, we find that non-topological stripes (corresponding to in-phase domain wall state) are indeed established due to enhanced antiferromagnetic interactions (as first speculated by Castro-Neto [8]). Yet, thus far the connection is more heuristic than rigorous.

Furthermore, after analyzing the effect higher order derivative terms in a gradient expansion of the Ginzburg-Landau free energy, Pryadko *et al.* argue that [6]: When there is no frustration, topological stripes are not established in the ground state. However they speculate that frustration, such as competing first and second neighbor interactions, or opposite sign terms in the gradient expansion of the Ginzburg-Landau model (*i.e.* below a Lifshitz point), can stabilize topological collinear domain walls. In other words, *topological stripes are a consequence of physics on short length scale, and they do not appear in a theory that considers only long-distance or low-energy physics.*

Pryadko *et al.* speculate that the missing frustrating ingredient may be due to inter-stripe interactions such as long range coulomb interactions which are expected to exist between the charged domain walls. Our analysis in this paper demonstrate that such interactions are not required. We have shown that local single stripe dynamic interactions, (albeit involving finite strength competing interactions, *i.e.*, expectantly beyond the reach of perturbative gradient expansion) are sufficient to realize both alternative possible topological magnetic order across the charge line.

## VI. ESTIMATE OF SPIN-WAVE VELOCITY

In this section, we use our microscopic domain wall model to estimate spin-wave velocity reduction

$$\alpha_v = \frac{v_\perp}{v_0}, \quad (46)$$

where  $v_\perp$  is the spin-wave velocity perpendicular to the stripes (*i.e.*, along the modulation direction), and  $v_0$  is the spin-wave velocity in the undoped parent antiferromagnetic material. Equivalently, it is the predicted spin-wave velocity anisotropy in stripes (where  $v_0$  is the same as the velocity along the stripes). Castro-Neto & Hone [7] were the first to point out that within the stripes model, one of the main effects of the hole rich lines would be to weaken the effective exchange interaction between spins on either side across the domain wall. Thus, a cardinal parameter in the model is the effective weakening factor of the magnetic interaction  $J_W$  across the stripes domain wall as compared with the Heisenberg interaction  $J$  within the hole free AFM regions (and hence along the stripes).

$$\alpha_J = \frac{J_W}{J} \quad (47)$$

The *key new ingredient is our analytical estimate of  $\alpha_J$* . Consequently, while previous model estimates always involved fitting of free parameters, we are able to estimate analytically the spin-wave velocity anisotropy (without any free parameters).

Neto&Hone [7] proposed an effective anisotropic Heisenberg model for describing the low temperature spin dynamics in a striped Cu-O plane. Within the anisotropic Heisenberg model [7], they derived the spin-wave velocity anisotropy

$$v_\perp \approx \sqrt{\frac{\alpha_J}{2}} v_0. \quad (48)$$

*i.e.*,  $\alpha_v = \sqrt{\frac{\alpha_J}{2}}$ . By fitting other consequences of their model to experimental results, Neto&Hone extracted the value

$$\alpha_J \approx 0.01.$$

The fitted value of  $\alpha_J$ , together with (48)  $\hbar v_\perp \approx 50 \text{ meV} \cdot \text{\AA}$ . As discussed by Tranquada *et al.* [21], this value is much too small to be compatible with inelastic neutron scattering experiments. It is further incompatible with the range of energies over which stripes incommensurability is observed.

Aiming specifically to model the interaction between narrow stripe AFM regions, Tworzydło *et al.* [22] made predictions based on models of coupled narrow spin ladders (e.g., 2-leg or 3-leg ladders). The resulting expressions for the spin wave velocity anisotropy were

$$\alpha_v = \begin{cases} \sqrt{\frac{2\alpha_J}{1+\alpha_J}} & \text{for 2-leg ladder} \\ \sqrt{\frac{3\alpha_J}{1+2\alpha_J}} & \text{for 3-leg ladder} \end{cases} \quad (49)$$

In terms of 2-leg ladder model, Tranquada *et al.* proclaimed to fit the experiments well with a value of

$$\alpha_J \approx 0.35.$$

giving

$$\alpha_v \approx 0.72$$

In principle, the ladder model results are quite sensitive to the width of the stripes (which affects the ladder spin gap magnitude). Yet accidentally, the above value of  $\alpha_J \approx 0.35$  would give  $\alpha_v \approx 0.78$  for 3-leg ladder, *i.e.*, practically the same as for 2-leg.

Our microscopic model is based solely on the local physics in the neighborhood of the hole line. As such, it is insensitive to details of the width of the AFM spin domains. We argue that, by definition, the energy difference between alternative spin configurations across the domain wall is a measure of the effective spin interaction across the domain wall in any appropriate low energy theory. Therefore, using our microscopic model calculation, we suggest that

$$J_W = -\Delta E(\delta) = E^{\text{in}} - E^{\text{anti}} \quad (50)$$

where  $\Delta E(\delta)$  is given in equation (40)

$$\Delta E(\delta) \approx -\frac{\varepsilon}{2} \left[ 1 - \left( \frac{\varepsilon}{t} \right) \right] (1 - 2\delta) + 2 \left( 2\delta - \frac{1}{2} \right) \varepsilon$$

(where as discussed previously,  $\varepsilon \approx J$ ). Thus we can calculate  $\alpha_J$  and then, following the anisotropic Heisenberg model reasoning of Castro-Neto & Hone, use (48) to calculate the spin-wave velocity anisotropy.

For the particular case of stripes observed in LaNdSr-CuO [1]  $\delta \approx 1/4$ , we obtain

$$J_W \approx \Delta E \left( \delta = \frac{1}{4} \right) \approx \frac{J}{4} \left[ 1 - \left( \frac{J}{t} \right) \right] \quad (51)$$

Substituting  $\frac{1}{3} > \frac{J}{t} > \frac{1}{10}$ , we obtain

$$0.17 < \alpha_J (\delta \approx 1/4) < 0.23 \quad (52)$$

Importantly, note that  $\alpha_J (\delta \approx 1/4)$  is rather insensitive to the variation of  $\frac{J}{t} < \frac{1}{3}$ . (where  $\delta \approx 1/4$  is the supposed electron filling fraction of the stripe domain walls in Copper-Oxides).

Using equation (48) thus give an estimate of

$$0.29 < \alpha_v < 0.34 \quad (53)$$

or using equation (49) give an estimate of

$$\begin{aligned} 0.67 < \alpha_v < 0.71 & \text{ for 2-leg ladder domains} \\ 0.74 < \alpha_v < 0.78 & \text{ for 3-leg ladder domains} \end{aligned} \quad (54)$$

which fit remarkably well with the experimentally deduced spin wave velocity inhibition  $0.60 < \alpha_v < 0.72$  in doped Copper-Oxides compared with the undoped parent AFM material [23]. Note that our estimate is obtained by directly substituting the experimental value of  $v_0$  into the analytical results for  $\alpha_J$  (using our model equation (40)) and for  $\alpha_v$  (from the ladder models [22] or the anisotropic Heisenberg model [7]), without any fitting of free parameters.

**Acknowledgments:** I thank Natan Andrei, Thierry Giamarchi, Baruch Horovitz, Efstratios Manousakis, John Tranquada, and particularly Steve Kivelson for fruitful discussions. This work was partly supported by the TMR#ERB4001GT97294 fellowship.

- [5] O. Zachar, S. A. Kivelson, and V. J. Emery, Phys. Rev. B **57**,1422 (1998).
- [6] Leonid P. Pryadko, Steven A. Kivelson, V. J. Emery, Yaroslav B. Bazaliy, Eugene A. Demler, Phys. Rev. B **60**,7541 (1999).
- [7] A. H. Castro Neto and D. Hone, Phys. Rev. Lett. **76**, 2165 (1996).
- [8] A. H. Castro Neto, Proceedings of the Euroconference on "Correlations in unconventional quantum liquids" in Zeitschrift fur Physik B - Condensed Matter (1997).
- [9] Chetan Nayak and Frank Wilczek, Phys. Rev. Lett. **78**,2465 (1997).
- [10] A. L. Chernyshev, A. H. Castro Neto, A. R. Bishop, cond-mat/9909128.
- [11] F.C. Zhang and T.M. Rice, Phys. Rev. B **37**, 3759 (1988).
- [12] Stephen Hellberg and E. Manousakis, Phys. Rev. Lett. **83**,132 (1999).
- [13] J. M. Tranquada, P. Wochner, A. R. Moodenbaugh, D. J. Buttrey, Phys. Rev. B **55**,6113 (1997).
- [14] O. Zachar, unpublished.
- [15] The image in figure-1a, where there are two anti-parallel spins with an empty site in between, may evoke contemplations of a super-exchange mechanism. But this is wrong, since the middle site double occupation is excluded (which is the essence of super-exchange).
- [16] E.W. Carlson, S.A. Kivelson, Z. Nussinov, V.J. Emery, Phys. Rev. B **57**,14704 (1998).
- [17] Clarence Zener, Phys. Rev. **82**,403 (1951).
- [18] A. Aurbach and B.E. Larson, Phys. Rev. Lett. **66**,2262 (1991).
- [19] Intuitively, it is expected that the net scattering due to spin exchange interaction are weaker for an anti-phase than an in-phase domain wall. Thus, among other things, it further indicates that the hole mobility favors an anti-phase domain wall.
- [20] S.A. Kivelson, V.J. Emery and H.Q. Lin, Phys. Rev. B **42**,6523 (1990); Oleg Tchernyshyov and Leonid P. Pryadko, cond-mat/0001068.
- [21] J.M. Tranquada, N. Ichikawa and S. Uchida, Phys. Rev. B **59**,14712 (1999).
- [22] Jakub Tworzydło, Osman Y. Osman, Coen N. A. van Duin, and Jan Zaanen, Phys. Rev. B **59**,115 (1999).
- [23] G. Aeppli *et al.* Phys. Rev. Lett. **62**,2052 (1989); S.M. Hayden *et al.* Phys. Rev. Lett. **66**,821 (1991).

- 
- [1] J. Tranquada *et al.*, *Nature* **375**, 561 (1995); J. Tranquada, *Physica C* **282-287**, 166 (1997).
  - [2] J. Zaanen and P. B. Littlewood, Phys. Rev. B **50**, 7222 (1994).
  - [3] The modulated antiferromagnetic order resulting from Hartree-Fock theory [2], of small doping away from half filling, which leads to diagonal spin stripes due to Fermi surface nesting instability. In that model the mechanism is spin driven and the charge ordering is secondary.
  - [4] V. J. Emery and S. A. Kivelson, *Physica C* **209**, 597 (1993); G. Seibold, C. Castellani, C. Di Castro, M. Grilli, Phys. Rev. B **58**,13506 (1998).